Kvantfysik Lecture Notes No. 4

In this installment of the lecture notes we make two general statements about the eigenstates of the time-independent Schrödinger equation. We then discuss the particle in the box. We then consider the free particle. We also include several appendices with some useful mathematics.

1 Two general statements about H eigenstates

1.1 Stationary states

Suppose that we have a normalized eigenstate of the time independent Schrödinger equation, $\psi(x)$ with energy eigenvalue E. Then the corresponding solution to the time dependent Schrödinger equation, $\Psi(x,t) = \exp(-iEt/\hbar)\psi(x)$ is a *stationary state*. If we consider the probability density $\rho(x,t)$ we find

$$\frac{\partial}{\partial t}\rho(x,t) = \frac{\partial}{\partial t}(\Psi^*\Psi) = \frac{\partial}{\partial t}(\psi(x)^*\psi(x)) = 0\,,$$

and so $\rho(x,t)$ is constant in time. Furthermore, if we consider the expectation value of any observable $\mathcal{O}$ that has no explicit time dependence, then

$$\frac{d}{dt}\langle\mathcal{O}\rangle = \int \frac{\partial}{\partial t}\left(\Psi^*\hat{\mathcal{O}}\,\Psi\right)\,dx = \int \frac{\partial}{\partial t}\left(\psi^*\hat{\mathcal{O}}\,\psi\right)\,dx = 0\,,$$

since none of the quantities in the final parentheses has any explicit time dependence. Hence all expectation values are constant in time. Notice the difference between this statement and the discussion in section 4 of the Lecture 3 notes. There we said that the time derivative of an expectation value is zero if the associated operator commutes with the Hamiltonian no matter what $\Psi(x,t)$ is. Here we are saying the time derivative is zero if $\Psi(x,t)$ is a stationary state *no matter what the operator* $\hat{\mathcal{O}}$ is.

1.2 Orthonormality of eigenstates

Let ψ_n be the complete set of normalized eigenstates of H with eigenvalues E_n. Consider then the integral,

$$\int \psi_n^* H\psi_m\,dx = \int (H\psi_n)^*\psi_m\,dx$$

where n and m label two different eigenstates ($n \neq m$) and we use that H is Hermitian. We can then replace H acting on the eigenstates with their respective eigenvalues to find

$$
\begin{aligned}
& \int \psi_n^* E_m \psi_m \, dx = \int (E_n \psi_n)^* \psi_m \, dx \\
\Rightarrow \qquad & E_m \int \psi_n^* \psi_m \, dx = E_n \int \psi_n^* \psi_m \, dx \qquad \text{since } E_n \text{ is real}
\end{aligned}
$$

Assuming that $E_n \neq E_m$, consistency requires that

$$\int \psi_n^* \psi_m \, dx = 0 \, .$$

Including the possibility of having $n = m$, we can write the orthonormality condition,

$$\int \psi_n^* \psi_m \, dx = \delta_{nm} \, ,$$

where δ_{nm} is the Kronecker δ-function with $\delta_{nm} = 1$ if $n = m$ and $\delta_{nm} = 0$ if $n \neq m$. A properly normalized general solution $\Psi(x,t)$ then satisfies

$$
\begin{aligned}
\int \Psi^* \Psi \, dx &= \int \sum_n c_n^* e^{+iE_n t/\hbar} \psi_n^* \sum_m c_m e^{-iE_m t/\hbar} \psi_m \, dx \\
&= \sum_{n,m} c_n^* c_m e^{+iE_n t/\hbar - iE_m t/\hbar} \int \psi_n^* \psi_m \, dx \\
&= \sum_{n,m} c_n^* c_m e^{+iE_n t/\hbar - iE_m t/\hbar} \delta_{nm} = \sum_n |c_n|^2 = 1 \, .
\end{aligned}
$$

$|c_n|^2$ is interpreted as the probability that the particle is in eigenstate n with energy E_n.

Note that if two independent eigenstates ψ_n and ψ_m have the same energy, $E_n = E_m$, the eigenstates are said to be *degenerate*. If these eigenstates are not orthogonal, one can always choose two linearly independent combinations of ψ_n and ψ_m which are orthogonal.

2 Infinite Square Well (or the Particle in a Box)

We are finally ready to consider our first physical system, a particle constrained to be in a one-dimensional box of length a. We assume that there are no forces on the particle while inside the box, but there is an infinite potential that prevents the particle from getting out, no matter what its energy. Hence, we write the potential as

$$
\begin{aligned}
V(x) &= 0 \qquad 0 \leq x \leq a \\
V(x) &= \infty \qquad x < 0 \text{ or } x > a
\end{aligned}
\tag{1}
$$

Here is a graph of the potential:

2.1 Eigenfunctions and eigenvalues

Let us now look for eigenfunctions (eigenstates), $\psi_n(x)$, and eigenvalues, E_n, of the Schrödinger equation for this potential. We first must establish boundary conditions. Since the particle is not allowed to leave the box, the probability density $\rho(x) = 0$ if $x < 0$ or $x > a$. Hence,

$$\psi_n(x) = 0 \qquad x > a \text{ or } x < 0\,.$$

Then the continuity of $\psi_n(x)$ gives the boundary conditions

$$\psi_n(0) = \psi_n(a) = 0.$$

In the region $0 \leq x \leq a$ the time independent Schrödinger equation is

$$E_n \psi_n(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_n(x)\,,$$

whose general solution is

$$\psi_n(x) = A_n \sin(k_n x) + B_n \cos(k_n x)$$

where we use that $\frac{d}{dx}\sin kx = k\cos kx$, $\frac{d}{dx}\cos kx = -k\sin kx$. Plugging this solution back into the Schrödinger equation, we find

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_n(x) = \frac{\hbar^2}{2m}k_n^2\psi_n(x) \qquad \Rightarrow \qquad E_n = \frac{k_n^2\hbar^2}{2m}$$

Now, $\sin(0) = 0$, $\cos(0) = 1$, therefore to be consistent with the boundary condition $\psi_n(0) = 0$, we have $B_n = 0$. We then have

$$\psi_n(a) = A_n \sin(k_n a) = 0,$$

which is satisfied if

$$k_n a = n\pi, \qquad n = 1, 2 \ldots.$$

$$\text{Hence} \quad k_n = \frac{n\pi}{a}, \qquad E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}.$$

Therefore, the energy levels are quantized!

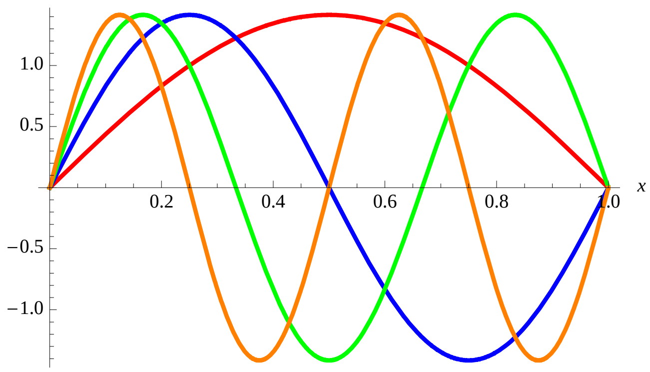


Figure 1: First four wave functions for a particle in a box

2.2 Normalizing the eigenfunctions (eigenstates)

We want normalized eigenfunctions so that we can properly compute probability densities and expectation values. For the ψ_n we find

$$\begin{aligned} 1 = \int \psi_n^* \psi_n \, dx &= \int_0^a |A_n|^2 \sin^2 \tfrac{n\pi x}{a} \, dx \\ &= \int_0^a |A_n|^2 \left(\tfrac{1}{2} - \tfrac{1}{2} \cos \tfrac{2n\pi x}{a} \right) dx = |A_n|^2 \frac{a}{2} + 0 \end{aligned}$$

$$A_n = \sqrt{\tfrac{2}{a}} \quad \text{up to an unobservable phase.}$$

2.3 The general state

The normalized states satisfy

$$\int \psi_n^* \psi_m \, dx = \int_0^a \psi_n^* \psi_m \, dx = \delta_{nm} \, ,$$

since $E_n \neq E_m$ if $n \neq m$. Any continuous function $\psi(x)$ with $\psi(0) = \psi(a) = 0$ can be written as

$$\psi(x) = \sum_{n=1}^{\infty} c_n \psi_n(x).$$

For any given $\psi(x)$ we can use the orthonormality of the eigenfunctions to find the coefficients c_n. To do this we compute the integral

$$\int \psi_n^* \psi \, dx = \int_0^a \psi_n^* \sum_m c_m \psi_m \, dx = \sum_m c_m \delta_{nm} = c_n$$

If $\psi(x)$ is properly normalized then the c_n satisfy

$$\sum_{n=1}^{\infty} |c_n|^2 = 1 \, .$$

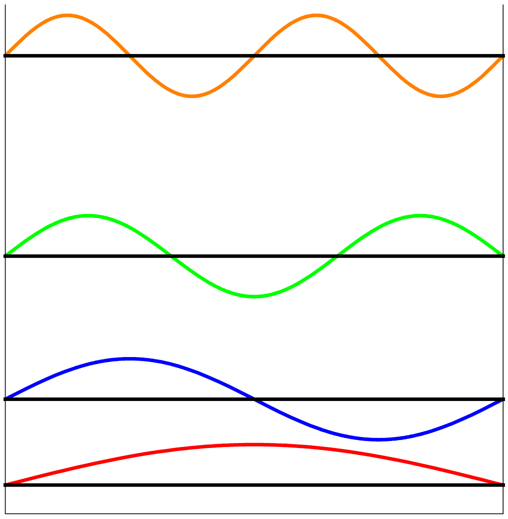


Figure 2: Another way to display the wavefunctions, where information about their energies is also included. Notice that the 1st and 3rd are even while the 2nd and 4th are odd.

Finding the c_n is crucial for finding the time evolution of the wave function If $\Psi(x,0) = \psi(x)$, then for arbitrary time t we have

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \, e^{-iE_n t/\hbar} \, \psi_n(x) \, .$$

2.4 Measurement of Energies:

A measurement of the energy will give one of the eigenvalues (otherwise, what's the point of saying the energies are quantized!). The probability for finding $E = E_n$ is $|c_n|^2$. Note that the normalization condition means that the sum of these probabilities is 1. Immediately after the measurement, the wavefunction collapses to one of the energy eigenstates, $\psi_n(x)$.

2.5 An example

Here is an example calculation:

$$\Psi(x,0) = \tfrac{1}{\sqrt{2}}\psi_1(x) + \tfrac{1}{\sqrt{2}}\psi_2(x)$$

$$c_1 = \tfrac{1}{\sqrt{2}}, \quad c_2 = \tfrac{1}{\sqrt{2}}, \quad c_n = 0, \; n > 2$$

$$\Psi(x,t) = \tfrac{1}{\sqrt{2}}\sqrt{\tfrac{2}{a}} \left(e^{-iE_1 t/\hbar} \sin \tfrac{\pi x}{a} + e^{-iE_2 t/\hbar} \sin \tfrac{2\pi x}{a} \right)$$

This is not a stationary state (the probability density $\Psi^*\Psi$ is not constant in t):

$$\begin{aligned}\Psi^*\Psi &= \frac{1}{a}\left(\sin^2\tfrac{\pi x}{a} + \sin^2\tfrac{2\pi x}{a} + \left[e^{i(E_2-E_1)t/\hbar} + e^{-i(E_2-E_1)t/\hbar}\right]\sin\tfrac{\pi x}{a}\sin\tfrac{2\pi x}{a}\right) \\ &= \frac{1}{a}\left(\sin^2\tfrac{\pi x}{a} + \sin^2\tfrac{2\pi x}{a} + 2\cos\tfrac{(E_2-E_1)t}{\hbar}\sin\tfrac{\pi x}{a}\sin\tfrac{2\pi x}{a}\right)\end{aligned}$$

To find $\langle x\rangle$ we will need the following integrals:

$$\begin{aligned}\int_0^a x\sin\tfrac{n\pi x}{a}\,dx &= -\frac{a}{n\pi}x\cos\tfrac{n\pi x}{a}\Big|_0^a + \frac{a}{n\pi}\int_0^a \cos\tfrac{n\pi x}{a}\,dx \\ &= -\frac{a^2}{n\pi}(-1)^n + \frac{a^2}{n^2\pi^2}\sin\tfrac{n\pi x}{a}\Big|_0^a = \frac{a^2}{n\pi}(-1)^{n+1} \qquad \boxed{\text{using } \sin n\pi = 0} \\ \int_0^a x\cos\tfrac{n\pi x}{a}\,dx &= \frac{a}{n\pi}x\sin\tfrac{n\pi x}{a}\Big|_0^a - \frac{a}{n\pi}\int_0^a \sin\tfrac{n\pi x}{a}\,dx \\ &= 0 + \frac{a^2}{n^2\pi^2}\cos\tfrac{n\pi x}{a}\Big|_0^a = \frac{a^2}{n^2\pi^2}\left((-1)^n - 1\right)\end{aligned}$$

We also have the trigonometric relation

$$\sin\tfrac{n\pi x}{a}\sin\tfrac{m\pi x}{a} = \tfrac{1}{2}\cos\tfrac{(n-m)\pi x}{a} - \tfrac{1}{2}\cos\tfrac{(n+m)\pi x}{a}$$

$$\Rightarrow \qquad x\Psi^*\Psi = \frac{x}{2a}\left(1 - \cos\tfrac{2\pi x}{a} + 1 - \cos\tfrac{4\pi x}{a} + 2\cos\tfrac{(E_2-E_1)t}{\hbar}\left(\cos\tfrac{\pi x}{a} - \cos\tfrac{3\pi x}{a}\right)\right)$$

$$\begin{aligned}\langle x\rangle &= \int_0^a \frac{x}{2a}\left(1 - \cos\tfrac{2\pi x}{a} + 1 - \cos\tfrac{4\pi x}{a} + 2\cos\tfrac{(E_2-E_1)t}{\hbar}\left(\cos\tfrac{\pi x}{a} - \cos\tfrac{3\pi x}{a}\right)\right)dx \\ &= \frac{1}{2a}\left(\frac{a^2}{2} - 0 + \frac{a^2}{2} - 0 + 2\cos\tfrac{(E_2-E_1)t}{\hbar}\left(-\frac{2a^2}{\pi^2} + \frac{2a^2}{9\pi^2}\right)\right) \\ &= \frac{a}{2} - \left(\frac{16}{9\pi^2}\right)a\cos\tfrac{(E_2-E_1)t}{\hbar} \qquad \boxed{\text{oscillates about the center, } \tfrac{a}{2}}\end{aligned}$$

$$\langle p\rangle = m\frac{d}{dt}\langle x\rangle = \frac{m(E_2-E_1)}{\hbar}\frac{16}{9\pi^2}a\sin\tfrac{(E_2-E_1)t}{\hbar} = \frac{8\hbar}{3a}\sin\tfrac{(E_2-E_1)t}{\hbar}$$

Question: Does $\frac{d}{dt}\langle p\rangle = \langle -\frac{\partial}{\partial x}V(x)\rangle$?
Answer: Yes, even though $\partial V = 0$ when $0 < x < a$, but $\frac{d}{dt}\langle p\rangle \neq 0$ when $0 < \langle x\rangle < a$. Is this a contradiction?

2.6 A first look at symmetries

Let us consider the same particle in the box potential, except now we replace the x coordinate with $x + a/2$. This shifts the potential in (1) to

$$\begin{aligned}V(x) &= 0 \qquad -\frac{a}{2} \le x \le \frac{a}{2} \\ V(x) &= \infty \qquad |x| > \frac{a}{2},\end{aligned}$$

giving a potential symmetric about $x = 0$, $V(-x) = V(x)$. The shift should have no effect on the energies and should only change the eigenfunctions by replacing x with $x + a/2$, $\psi_n(x) \to \psi_n(x + a/2)$. Thus, the normalized wave-functions become

$$\Rightarrow \qquad \psi_n(x) \to \psi_n(x + a/2) = \sqrt{\tfrac{2}{a}} \sin\left(\tfrac{n\pi}{a}(x + a/2)\right) = \sqrt{\tfrac{2}{a}} \sin\left(\tfrac{n\pi}{a}x + \tfrac{n\pi}{2}\right)$$

$$\begin{aligned} &= +\sqrt{\tfrac{2}{a}} \cos \tfrac{n\pi x}{a} && n = 1 \bmod 4 \\ &= -\sqrt{\tfrac{2}{a}} \sin \tfrac{n\pi x}{a} && n = 2 \bmod 4 \\ &= -\sqrt{\tfrac{2}{a}} \cos \tfrac{n\pi x}{a} && n = 3 \bmod 4 \\ &= +\sqrt{\tfrac{2}{a}} \sin \tfrac{n\pi x}{a} && n = 0 \bmod 4 \end{aligned}$$

(Note that $n = p \bmod 4$ if $n = p + 4m$ where m is any integer.) If we absorb the minus signs into the definitions of the wave-functions, we are left with two types of solutions,

$$\begin{aligned} \psi_n(x) &= \sqrt{\tfrac{2}{a}} \cos \tfrac{n\pi x}{a} && n \text{ odd} \\ \psi_n(x) &= \sqrt{\tfrac{2}{a}} \sin \tfrac{n\pi x}{a} && n \text{ even}\,. \end{aligned} \tag{2}$$

These can also be defined as

$$\begin{aligned} \psi_{n+}(x) &= \sqrt{\tfrac{2}{a}} \cos \tfrac{(2n-1)\pi x}{a} && n = 1, 2, \ldots \\ \psi_{n-}(x) &= \sqrt{\tfrac{2}{a}} \sin \tfrac{(2n)\pi x}{a} && n = 1, 2, \ldots\,. \end{aligned} \tag{3}$$

The first (second) set of solutions is even (odd) under $x \to -x$, $\psi_{n\pm}(-x) = \pm\psi_{n\pm}(x)$.

2.7 Parity operator Π

Consider the *parity* operator, whose action on a wave-function is

$$\Pi\, \psi(x) = \psi(-x)$$

Hence, ψ_{n+} and ψ_{n-} are eigenfunctions of Π with eigenvalues ± 1. These are the only possible eigenvalues since $\Pi^2 = 1$. Next consider Π and H both acting on the wave-function:

$$\begin{aligned} \Pi\, H\, \psi(x) &= \Pi \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right) \psi(x) \\ &= \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(-x)\right) \psi(-x) && \boxed{\Pi \text{ changes all signs of } x \text{ to the right}} \\ &= \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(-x)\right) \Pi\, \psi(x) \end{aligned}$$

Thus, if $V(-x) = V(x)$ then $\Pi\, H = H\, \Pi$, that is $[\Pi, H] = 0$, (Π commutes with H). If $[\Pi, H] \neq 0$, then $\psi(x)$ cannot be an eigenfunction for both operators. To see why, let us suppose that it could be an eigenfunction for both, with eigenvalue $\alpha = \pm 1$ for Π and E for H. then

$$
\begin{aligned}
(\Pi\, H \,-\, H\, \Pi)\psi \,=\, (\Pi\, E \,-\, H\, \alpha)\psi \;&=\; (E\, \Pi \,-\, \alpha\, H)\psi \qquad \boxed{\text{ops. commute with numbers}} \\
&=\; (E\, \alpha \,-\, \alpha\, E)\psi \,=\, 0
\end{aligned}
$$

But this is a contradiction, because by assumption

$$
[\Pi, H]\psi(x) = (V(-x) - V(x))\psi(-x) \neq 0.
$$

Operators that commute can have simultaneous eigenfunctions. For the symmetric version of the infinite square well, the even and odd wave-functions are also eigenfunctions of H. We also have that

$$
\frac{d}{dt}\langle \Pi \rangle = \frac{i}{\hbar}\langle [H, \Pi] \rangle = 0\,.
$$

This means that parity is conserved.

3 The free particle

Let us now assume that $V(x) = V_0$ for all x, where V_0 is a constant. This corresponds to a free particle (a particle with no forces acting on it.) Perhaps surprisingly, this is a somewhat delicate problem.

The time independent Schrödinger equation is

$$
E\psi(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V_0\,\psi(x)
$$

If $E > V_0$ then there are two independent solutions known as *plane waves*

$$
\psi(x) = A\, e^{ikx}\,, \quad B\, e^{-ikx} \qquad k = \frac{\sqrt{2m(E - V_0)}}{\hbar}\,.
$$

One eigenstate corresponds to a wave traveling in the positive direction and the other is a wave traveling in the negative direction.

We can also write a general plane wave as $\psi(x) = A\, e^{ipx/\hbar}$, where p can have any real value, and which has energy eigenvalue $E(p) = \frac{p^2}{2m} + V_0$. In other words, the plane waves are also eigenfunctions of the momentum operator $\hat{p}$. From our discussion in the previous lecture, this means that $[\hat{p}, H] = 0$, as you can readily check since V has no x dependence. For a given eigenvalue of H, there are two possible choices for p, $\pm|p|$, hence the eigenstates are doubly degenerate.

As an aside, suppose that we were to look for solutions where $E < V_0$. Then the solutions to the Schrödinger equation are

$$\psi(x) = Ae^{\kappa x}, \quad Be^{-\kappa x} \qquad\qquad \text{where } \kappa = \frac{\sqrt{2m(V_0 - E)}}{\hbar}\,.$$

But neither of these solutions are normalizable; the first wave function blows up exponentially as x approaches $+\infty$, while the second blows up as x approaches $-\infty$, so we drop them (although we will have use for these solutions later).

However, even the plane waves are not normalizable as we can easily check:

$$\int_{-\infty}^{\infty} \psi^*(x)\,\psi(x)\,dx = \int_{-\infty}^{\infty} A^*\,e^{-ipx/\hbar}\,A\,e^{+ipx/\hbar}\,dx = |A|^2 \int_{-\infty}^{\infty} dx = \infty$$

for any nonzero A. Hence we are unable to choose an A such that the integral is 1. We now discuss two ways to get around this problem.

3.1 The particle on a circle

The infinity occurs because of the infinite length along the x direction. So one thing we could try is to cut off this length at some large, but finite value. One way to do this is to put the particle into a box of size L. However, we already know the eigenfunctions, they are

$$\psi(x) = \sqrt{\frac{2}{L}}\sin\frac{px}{\hbar} = \frac{i}{\sqrt{2L}}\left(e^{-ipx/\hbar} - e^{ipx/\hbar}\right)$$

where the p are quantized to be $p = \pi\hbar n/L$ for $n \geq 1$. If L is very large, then the spacing between the allowed values of p becomes very small and p becomes almost continuous. However, the problem with these eigenstates is that the eigenfunctions are standing waves, while we would like to have traveling waves.

An alternative to the box is to put the position x on a circle of circumference L. What this means is that if we shift x by L, we come back to the same point. The wave function should be single valued on the circle, which means that $\psi(x+L) = \psi(x)$. Hence, the allowed p are quantized to enforce this condition. If

$$\psi(x) = A\,e^{ipx/\hbar} = \psi(x+L) = A\,e^{ip(x+L)/\hbar}\,,$$

then $pL/\hbar = 2\pi n$ where n is any integer (not just positive integers) since $e^{2\pi i n} = 1$. This wave function is normalizable because now we should only integrate $\psi^*\psi$ from 0 to L (we only integrate over the circle once). Hence, we have

$$\int_0^L \psi^*(x)\,\psi(x)\,dx = |A|^2 \int_0^L dx = |A|^2\,L$$

and so $A = 1/\sqrt{L}$ up to a phase. Note that $Ae^{ipx/\hbar}$ and $Ae^{-ipx/\hbar}$ are distinct eigenfunctions on the circle, and so the circle can have traveling waves. If we now take L to be very large, then the allowed p approach a continuous distribution, but our wave functions are still normalizable. If L is very large, say the circumference of the earth, then this is very close to having the length be infinite. So even though the original wave functions were not normalizable, it did not take much to make them normalizable. For this reason, plane waves are said to be *plane wave normalizable* to distinguish them from the far worse case that one typically encounters for nonnormalizable wave functions.

3.2 Wavepackets

The momentum eigenstates have $\psi^*(x)\psi(x)$ constant in x, meaning that the particle has equal probability to be anywhere. Thus $\sigma_x = \infty$, which is to be expected from Heisenberg uncertainty, since the plane wave is an exact eigenstate of $\hat{p}$ and so $\sigma_p = 0$. This is the source of the problem of the nonnormalizability of the plane waves.

Therefore, an alternative procedure is to give up having exact eigenstates of the Hamiltonian, instead choosing the wave functions to be close to eigenstates. In this case, we can have a large, but finite σ_x. The most common way to modify the wave function is to multiply it by a Gaussian with a large Δx. Choosing $p = p_0$, we have

$$\psi(x) = \frac{1}{\sqrt{\Delta x\sqrt{2\pi}}}\,\exp\left(-\frac{x^2}{4\,\Delta x^2}\right)\,e^{ip_0x/\hbar}$$

where the normalization factor is derived in appendix A.1. This wave function is an example of a *wave packet*[1].

Since this wave function is not an eigenfunction of H, it is not a stationary state. To see how it evolves, we have to write $\psi(x)$ in terms of the eigenfunctions. We do this by taking the Fourier transform of $\psi(x)$. In appendix A.4 we review Fourier transforms and explicitly compute it for a gaussian. Here,

[1]The rest of this section has some fairly detailed and advanced mathematics. If you want you can skip to the result (4) for the probability density and the discussion afterward.

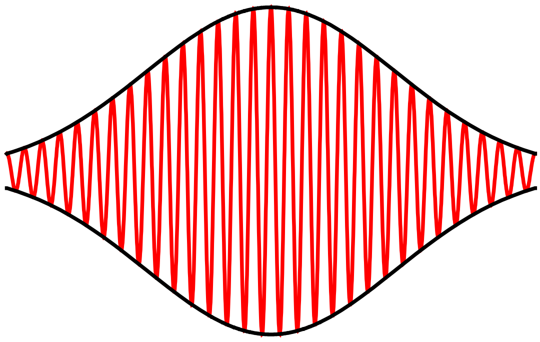


Figure 3: The real part of a plane wave slowly modulated by a Gaussian.

we have an extra factor of $e^{ip_0 x/\hbar}$ as compared to A.4, which shifts p in $\phi(p)$ by $-p_0$. Hence,

$$\phi(p) = \sqrt{\Delta x \sqrt{2\pi}} \exp\left(-(p-p_0)^2 (\Delta x)^2/\hbar^2\right) .$$

When we transform back, we have

$$\psi(x) = \int \frac{dp}{2\pi\hbar}\, e^{ipx/\hbar} \phi(p) \,.$$

But what we have done is written $\psi(x)$ as an integral over the eigenfunctions e^{ipx}, weighted by the coefficients $\phi(p)$, and so the full time dependent wave function is

$$\Psi(x,t) = e^{-iV_0 t/\hbar} \int \frac{dp}{2\pi\hbar}\, e^{ipx/\hbar} \exp\left(-i\,\frac{p^2}{2m\hbar}\,t\right) \phi(p) \,.$$

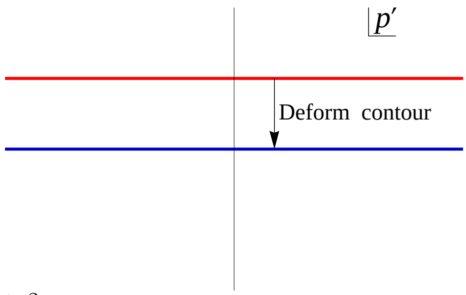
Explicitly writing out all terms and completing the square we have

$$\begin{aligned}\Psi(x,t) \;\; &= \;\; e^{-iV_0 t/\hbar} \sqrt{\Delta x \sqrt{2\pi}} \int \frac{dp}{2\pi\hbar} \exp\left(-\left((\Delta x)^2/\hbar^2 + \frac{it}{2m\hbar}\right)\left(p - \frac{p_0 (\Delta x)^2 + ix\,\hbar/2}{(\Delta x)^2 + \frac{it\hbar}{2m}}\right)^2\right) \times \\ &\times \exp\left(-\frac{\frac{it}{2m\hbar}(\Delta x)^2\, p_0^2}{(\Delta x)^2 + \frac{it\hbar}{2m}}\right) \exp\left(-\frac{1}{4(\Delta x)^2 + \frac{2it\hbar}{m})}\,x^2 + i\,\frac{(\Delta x)^2}{(\Delta x)^2 + \frac{it\hbar}{2m}}\,\frac{p_0 x}{\hbar}\right)\end{aligned}$$

Now we let p' be

$$p' = p - \frac{p_0(\Delta x)^2 + ix\,\hbar/2}{(\Delta x)^2 + \frac{it\hbar}{2m}}$$

and you can see for general x and t that p' will have a constant imaginary part over the integration region. This is shown as the red contour in the figure. However, the contour can be deformed so that the imaginary part is zero, without changing the value of the integral (the blue contour).[2] Hence the new integral is



$$\Psi(x,t) = e^{-iV_0t/\hbar}\sqrt{\Delta x\sqrt{2\pi}}\exp\left(-\frac{\frac{it}{2m\hbar}(\Delta x)^2 p_0^2}{(\Delta x)^2+\frac{it\hbar}{2m}}\right)\exp\left(-\frac{1}{4(\Delta x)^2+\frac{2it\hbar}{m})}x^2+i\frac{(\Delta x)^2}{(\Delta x)^2+\frac{it\hbar}{2m}}\frac{p_0x}{\hbar}\right)$$
$$\times\int_{-\infty}^{\infty}\frac{dp'}{2\pi\hbar}\exp\left(-\left((\Delta x)^2/\hbar^2+\frac{it}{2m\hbar}\right)(p')^2\right)$$

We can actually do this integral since it still has a Gaussian form, albeit a strange one since the coefficient of $(p')^2$ in the exponent is a complex number. But otherwise the rules for Gaussian integration apply (see A.1) and we find

$$\Psi(x,t) = e^{-iV_0t/\hbar}\sqrt{\frac{\Delta x}{\sqrt{2\pi}\left((\Delta x)^2+\frac{it\hbar}{2m}\right)}}\exp\left(-\frac{\frac{it}{2m\hbar}(\Delta x)^2 p_0^2}{(\Delta x)^2+\frac{it\hbar}{2m}}\right)\times$$
$$\exp\left(-\frac{1}{4(\Delta x)^2+\frac{2it\hbar}{m}}x^2+i\frac{(\Delta x)^2}{(\Delta x)^2+\frac{it\hbar}{2m}}\frac{p_0x}{\hbar}\right).$$

The probability density is then

$$\Psi^*\Psi = \frac{\Delta x}{\sqrt{2\pi\left((\Delta x)^4+\frac{t^2\hbar^2}{4m^2}\right)}}\exp\left(-\frac{\frac{t^2}{2m^2}(\Delta x)^2 p_0^2}{(\Delta x)^4+\frac{t^2\hbar^2}{4m^2}}\right)$$
$$\times\exp\left(-\frac{(\Delta x)^2}{2\left((\Delta x)^4+\frac{t^2\hbar^2}{4m^2}\right)}x^2+\frac{\frac{t}{m}(\Delta x)^2}{(\Delta x)^4+\frac{t^2\hbar^2}{4m^2}}p_0x\right)$$

$$= \frac{\Delta x}{\sqrt{2\pi\left((\Delta x)^4+\frac{t^2\hbar^2}{4m^2}\right)}}\exp\left(-\frac{(\Delta x)^2}{2\left((\Delta x)^4+\frac{t^2\hbar^2}{4m^2}\right)}\left(x-\frac{p_0}{m}t\right)^2\right) \quad (4)$$

We note two things about this expression. First, the peak, which is where the probability density is highest, is moving with velocity $v = p_0/m$. Notice

[2] You will learn why this is true if you ever take a mathematics course on complex analysis.

that this is the classical velocity of a particle with momentum p_0, the center of the Gaussian in p space. The second thing is that the width of the wave packet, σ_x, is spreading in time,

$$\sigma_x = \sqrt{\Delta x^2 + \frac{t^2\hbar^2}{4m^2\Delta x^2}}\,.$$

This is called *spreading of the wave packet*, naturally. We can get a better understanding for this by rewriting σ_x as

$$\sigma_x = \sqrt{\Delta x^2 + \frac{\sigma_p^2}{m^2}\,t^2}$$

where we used the result for σ_p at the very end of A.4. Note that σ_p/m is the uncertainty in the velocity of the particle. If there is an uncertainty in the velocity, then there is an additional uncertainty in the position of the particle after a time t, $\sigma_p\,t/m$, as the particle moves to a new position. This uncertainty is independent from the original uncertainty Δx. If two sources of a standard deviation are independent of each other, then the total standard deviation is found by taking the square root of the sum of their squares.

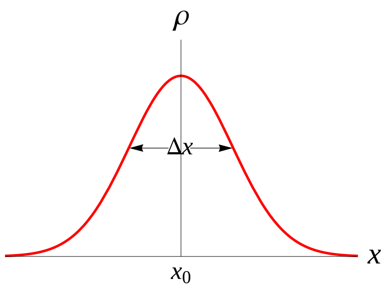
A Some useful mathematics

A.1 Gaussian distribution (bell curve)

Let the wave function and probability density at fixed time be

$$\psi(x) = A\,\exp\left(-\frac{(x-x_0)^2}{4\,\Delta x^2}\right)$$

$$\rho(x) = |A|^2\,\exp\left(-\frac{(x-x_0)^2}{2\,\Delta x^2}\right)$$



The density $\rho(x)$ is shown in the figure. The width of the Gaussian is Δx and it is centered at x_0. Choose A so that the wave function is properly normalized:

$$\int \psi^*\psi\,dx \;=\; |A|^2\int_{-\infty}^{\infty}\exp\left(-\frac{(x-x_0)^2}{2\,\Delta x^2}\right)dx = |A|^2\,\Delta x\,\sqrt{2\pi}$$

$$\Rightarrow \qquad A = \frac{1}{\sqrt{\Delta x\,\sqrt{2\pi}}}\,.$$

The standard deviation is found as follows:

$$\begin{aligned}\langle x\rangle &= \frac{\int \psi^* \, x \, \psi \, dx}{\int \psi^*, \psi \, dx} = \frac{1}{\Delta x\,\sqrt{2\pi}} \int_{-\infty}^{\infty} x \, \exp\left(-\frac{(x-x_0)^2}{2\,\Delta x^2}\right) dx \\ &= \frac{1}{\Delta x\,\sqrt{2\pi}} \int_{-\infty}^{\infty} (x' + x_0) \, \exp\left(-\frac{(x')^2}{2\,\Delta x^2}\right) dx' = x_0 \qquad \Leftarrow \boxed{\text{Change int. vars.}}\end{aligned}$$

$$\begin{aligned}\langle x^2\rangle &= \frac{\int \psi^* \, x^2 \, \psi \, dx}{\int \psi^*, \psi \, dx} = \frac{1}{\Delta x\,\sqrt{2\pi}} \int_{-\infty}^{\infty} x^2 \, \exp\left(-\frac{(x-x_0)^2}{2\,\Delta x^2}\right) dx \\ &= \frac{1}{\Delta x\,\sqrt{2\pi}} \int_{-\infty}^{\infty} ((x')^2 + 2x'x_0 + x_0^2) \, \exp\left(-\frac{(x')^2}{2\,\Delta x^2}\right) dx' \qquad \Leftarrow \boxed{\text{Change int. vars.}} \\ &= \frac{1}{\Delta x\,\sqrt{2\pi}} \left((\Delta x)^3\sqrt{2\pi} + 0 + x_0^2\,\Delta x\,\sqrt{2\pi}\right) = (\Delta x)^2 + x_0^2\end{aligned}$$

$$\sigma_x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \Delta x$$

A.2 The Dirac δ-function (a very useful function):

The Dirac δ-function, $\delta(x)$, has the following properties

$$\begin{aligned}\delta(x) &= 0 \qquad x \neq 0 \\ \delta(x) &= \infty \qquad x = 0 \\ \int_a^b \delta(x)\,dx &= 1 \qquad a < 0 \text{ and } b > 0 \\ &= 0 \qquad \text{otherwise}\end{aligned}$$

If we change variables to $x = ay$, we find

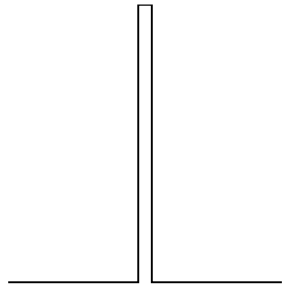
$$\begin{aligned}&\int_{-\infty}^{\infty} \delta(x)\,dx = \int_{-\infty}^{\infty} \delta(a\,y)\,a\,dy = a\int_{-\infty}^{\infty} \delta(a\,y)\,dy \\ \Rightarrow \qquad &\delta(a\,y) = \frac{1}{a}\,\delta(y)\end{aligned}$$

We also have

$$\int_a^b f(x)\,\delta(x)\,dx = \int_a^b f(0)\,\delta(x)\,dx = f(0)\int_a^b \delta(x)\,dx = f(0) \qquad a < 0 \text{ and } b > 0$$

There are several ways to define the function. Here's one:

$$\left.\begin{array}{rcll} \delta(x) & = & 0 & x < -\frac{\epsilon}{2} \text{ or } x > +\frac{\epsilon}{2} \\ \delta(x) & = & \frac{1}{\epsilon} & -\frac{\epsilon}{2} \le x \le +\frac{\epsilon}{2} \end{array}\right\} \text{limit } \epsilon \to 0$$

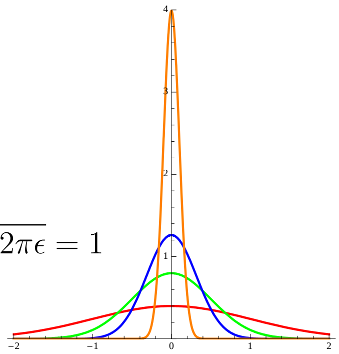


$$\int \delta(x)\, dx = \frac{1}{\epsilon}\int_{-\epsilon/2}^{\epsilon/2} dx = \frac{1}{\epsilon}\epsilon = 1$$

Here's another, where we use a gaussian:

$$\delta(x) = \lim_{\epsilon \to 0} \frac{1}{\sqrt{2\pi\epsilon}} \exp\left(-\frac{x^2}{2\epsilon}\right)$$

$$\int \delta(x)\, dx = \frac{1}{\sqrt{2\pi\epsilon}} \int_{-\infty}^{\infty} \exp\left(-\frac{x^2}{2\epsilon}\right) dx = \frac{1}{\sqrt{2\pi\epsilon}}\sqrt{2\pi\epsilon} = 1$$



Taking the limit on the gaussian

A.3 Integrating over plane-waves

Here we show a relation between plane-waves and the δ-function:

$$\begin{aligned} \int e^{ikx}\, dk &\Rightarrow \lim_{\epsilon \to 0} \int e^{ikx - \epsilon k^2/2}\, dk \\ &= \lim_{\epsilon \to 0} \int e^{-\epsilon(k - ix/\epsilon)^2/2 - x^2/(2\epsilon)}\, dk \qquad \Leftarrow \boxed{\text{complete the square}} \\ &= \lim_{\epsilon \to 0} \int_{-\infty - ix/\epsilon}^{\infty - ix/\epsilon} e^{-\epsilon k'^2/2 - x^2/(2\epsilon)}\, dk' \qquad \Leftarrow \boxed{\text{shift integration variables}} \\ &= \lim_{\epsilon \to 0} \int_{-\infty}^{\infty} e^{-\epsilon k'^2/2 - x^2/(2\epsilon)}\, dk' \qquad \Leftarrow \boxed{\text{deform the integration contour}} \\ &= \lim_{\epsilon \to 0} \frac{\sqrt{2\pi}}{\sqrt{\epsilon}} \exp\left(-\frac{x^2}{2\epsilon}\right) = 2\pi\, \delta(x) \end{aligned}$$

A.4 Fourier transforms

The fourier transform of a function $f(x)$ is given by

$$\tilde{f}(k) \equiv \int_{-\infty}^{\infty} dx\, e^{-ikx} f(x)\,.$$

Recall that $e^{ikx} = \cos kx + i \sin kx$. The inverse transform is then

$$\begin{aligned}
\int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ikx} \tilde{f}(k) &= \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ikx} \int_{-\infty}^{\infty} dx' e^{-ikx'} f(x') \\
&= \int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ikx} e^{-ikx'} f(x') \qquad \Leftarrow \boxed{\text{Reverse order of integration}} \\
&= \int_{-\infty}^{\infty} dx'\, \delta(x-x')\, f(x') \Leftarrow \boxed{\text{Use result from A.3}} \\
&= f(x)
\end{aligned}$$

If we express the transform in terms of $p = k\hbar$, then changing variables

$$\begin{aligned}
\tilde{f}(p) &\equiv \int_{-\infty}^{\infty} dx\, e^{-ipx/\hbar} f(x)\,. \\
f(x) &= \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} e^{ipx/\hbar} \tilde{f}(p)
\end{aligned}$$

where we have used that $dp = \hbar\, dk$.

The Fourier transform of the gaussian wave function is

$$\begin{aligned}
\phi(p) &= \int_{-\infty}^{\infty} dx\, e^{-ipx/\hbar} A \exp\left(-\frac{(x-x_0)^2}{4\,\Delta x^2}\right) dx \qquad \boxed{\text{complete the square}} \\
&= \frac{1}{\sqrt{\Delta x \sqrt{2\pi}}} \int_{-\infty}^{\infty} dx \exp\left(-\frac{(x - x_0 + 2ip(\Delta x)^2/\hbar)^2}{4\,\Delta x^2} - p^2(\Delta x)^2/\hbar^2 - ipx_0/\hbar\right) \\
&= \frac{1}{\sqrt{\Delta x \sqrt{2\pi}}} \int_{-\infty}^{\infty} dx' \exp\left(-\frac{(x')^2}{4\,\Delta x^2} - p^2(\Delta x)^2/\hbar^2 - ipx_0/\hbar\right) \Leftarrow \boxed{\text{shift int. vars. and deform}} \\
&= \sqrt{\Delta x \sqrt{2\pi}} e^{-ipx_0/\hbar} \exp\left(-p^2(\Delta x)^2/\hbar^2\right)
\end{aligned}$$

Comparing with the result for σ_x (see sec. A.1) we see that

$$\sigma_p = \frac{\hbar}{2\Delta x} \qquad \Rightarrow \qquad \sigma_x \sigma_p = \frac{\hbar}{2}\,. \qquad \boxed{\text{Consistent with Heisenberg Uncertainty}}$$